

**HIGH PRODUCTION VOLUME (HPV)**

**CHALLENGE PROGRAM**

**TEST PLAN**

**For**

**Thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide**

**Prepared by  
The American Chemistry Council  
Petroleum Additives Panel  
Health, Environmental, and Regulatory Task Group**

**August 8, 2003**

**LIST OF MEMBER COMPANIES IN THE  
HEALTH, ENVIRONMENTAL AND REGULATORY TASK GROUP**

The Health, Environmental, and Regulatory Task Group (HERTG) of the American Chemistry Council Petroleum Additives Panel includes the following member companies:

BP plc

Chevron Oronite Company, LLC

Crompton Corporation

Ethyl Corporation

ExxonMobil Chemical Company

Ferro Corporation

Infineum

The Lubrizol Corporation

Rhein Chemie Corporation

Rhodia, Inc. (formerly Albright & Wilson Americas Inc.)

## 1.0 INTRODUCTION

In March 1999, the American Chemistry Council (formerly the Chemical Manufacturers Association) Petroleum Additives Panel Health, Environmental, and Regulatory Task Group (HERTG), and its participating member companies committed to address data needs for certain chemicals listed under the Environmental Protection Agency (EPA) High Production Volume (HPV) Chemical Challenge Program. This test plan follows up on that commitment. Specifically, this test plan sets forth how the HERTG intends to address testing information for thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide, CAS Number: 18760-44-6.

In preparing this test plan the following steps were undertaken:

Step 1: A review of the literature and confidential company data was conducted on the physicochemical properties, mammalian toxicity endpoints, and environmental fate and effects for thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide, using its CAS number, CAS name, and synonyms. Searches included the following sources: MEDLINE, BIOSIS, CANCERLIT, CAPLUS, CHEMLIST, EMBASE, HSDB, RTECS, EMIC, and TOXLINE databases; the TSCATS database for relevant unpublished studies on these chemicals; and standard handbooks and databases (e.g., Sax, CRC Handbook on Chemicals, IUCLID, Merck Index, and other references) for physicochemical properties.

Step 2: The compiled data was evaluated for adequacy in accordance with the EPA guidance documentation.

## 2.0 GENERAL SUBSTANCE INFORMATION

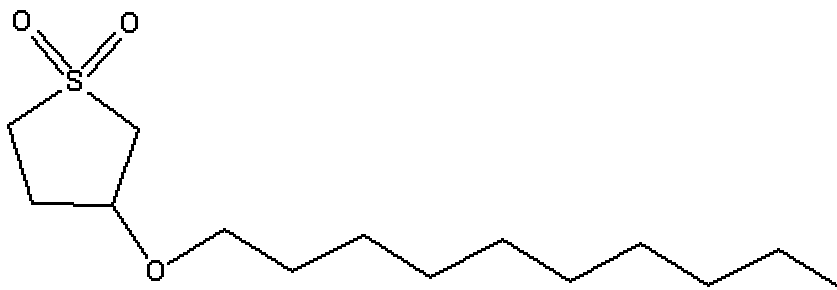
Chemical Name: thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide

Chemical Abstract Service Registry Number: CAS No.: 18760-44-6

Molecular Formula:  $C_{14}H_{28}O_3S$

Molecular Weight: 276.4

Structural Diagram:



**thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide**  
**CAS No.: 18760-44-6**

### **3.0 USE AND EXPOSURE INFORMATION**

The substance 2- thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide is a lubricating additive in many types of internal combustion engine oils, automatic transmission fluids, and hydraulic fluids. This component is generally blended into finished oils and fluids where the typical concentration is less than 1 wt.% depending on the application.

The substance 2- thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide is manufactured and blended into additive packages at plants owned by one or more members of the HERTG. Finished lubricants are blended at facilities owned by our customers. Additive packages are shipped to customers in bulk in ships, isocontainers, railroad tank cars, tank trucks or in 55-gallon steel drums. The bulk additive packages are stored in bulk storage tanks at the customer blending sites. Finished oils are blended by pumping the lubricating oil blend stocks and the additive package from their storage tanks through computer controlled valves that meter the precise delivery of the components into a blending tank. After blending, the finished lubricant products are sold in bulk and shipped in tank trucks to large industrial users, such as manufacturing facilities and facilities that service truck fleets and passenger motor vehicles. Finished lubricants are also packaged into 55-gallon drums, 5-gallon pails, and one-gallon and one-quart containers for sale to smaller industrial users. Sales of lubricants in one-gallon and one-quart containers to consumers at service stations or retail specialty stores also occur.

Based on these uses, the potentially exposed populations include (1) workers involved in the manufacture of 2- thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide, blending this component into additive packages, and blending the additive packages into finished lubricants; (2) quality assurance workers who sample and analyze these products to ensure that they meet specifications; (3) workers involved in the transfer and transport of 2- thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide, additive packages or finished lubricants that contain this component; (4) mechanics who may come into contact with both fresh and used lubricants while working on engines or equipment; (5) gasoline station attendants and consumers who may periodically add lubricating oil to automotive crankcases; and (6) consumers who may change their own automotive engine oil. The most likely route of human exposure for these substances is through dermal contact. The most likely source of environmental exposure is accidental spills at manufacturing sites or during transport.

**TABLE 1**  
**SUMMARY TABLE OF AVAILABLE DATA**

<b>CAS No.: 18760-44-6</b>	<b>Study Date</b>	<b>Study Results</b>	<b>Data Acceptable</b>
<b>Physical/Chemical Characteristics</b>			
<i>Melting Point</i>		Not Applicable	-
<i>Boiling Point</i>		No Data Located	-
<i>Vapor Pressure</i>		No Data Located	-
<i>Partition Coefficient</i>		No Data Located	-
<i>Water Solubility</i>	2002	54 mg/L at 20°C	Yes
<b>Environmental Fate</b>			
<i>Photodegradation</i>		No Data Located	-
<i>Hydrolysis</i>		No Data Located	-
<i>Fugacity</i>		No Data Located	-
<i>Biodegradation</i>	1997	9.6% at 28 days	Yes
<b>Ecotoxicity</b>			
<i>Acute Toxicity to Algae</i>	2002	EL <sub>50</sub> (72 hrs) = 3.5 mg/L WAF NOEL = 0.313 mg/L WAF	Yes
<i>Acute Toxicity to Invertebrates</i>		No Data Located	-
<i>Acute Toxicity to Fish</i>		No Data Located	-
<b>Mammalian Toxicity</b>			
<i>Acute Toxicity</i>	1975 1975	Rat Oral LD <sub>50</sub> >10 g/kg Rabbit Dermal LD <sub>50</sub> between 4 and 8 g/kg	Yes Yes
<i>Repeat Dose Toxicity</i>		No Data Located	-
<i>Developmental Toxicity</i>		No Data Located	-
<i>Reproductive Toxicity</i>		No Data Located	-
<b>Genetic Toxicity</b>			
<i>Gene Mutation</i>	1980	Not Mutagenic	Yes
<i>Chromosomal Aberration</i>		No Data Located	-

TABLE 2

## SUMMARY TABLE OF PROPOSED TESTING

Based on the data availability indicated in the above “Summary Table of Available Data” the following HPV Testing is proposed:

CAS No.: 18760-44-6	Testing Required	OECD Test Guideline or Testing Model Proposed
<b>Physical/Chemical Characteristics</b>		
<i>Melting Point</i>	Not Applicable	Not Applicable
<i>Boiling Point</i>	Yes	103
<i>Vapor Pressure</i>	Yes	104
<i>Partition Coefficient</i>	Yes	117
<i>Water Solubility</i>	No	-
<b>Environmental Fate</b>		
<i>Photodegradation</i>	Yes	AOPWIN Model
<i>Hydrolysis</i>	No	Technical Discussion
<i>Fugacity</i>	Yes	Fugacity Level 1 Type Model
<i>Biodegradation</i>	No	-
<b>Ecotoxicity</b>		
<i>Acute Toxicity to Algae</i>	No	-
<i>Acute Toxicity to Invertebrates</i>	Yes	OECD 202
<i>Acute Toxicity to Fish</i>	Yes	OECD 203
<b>Mammalian Toxicity</b>		
<i>Acute Toxicity</i>	No	-
<i>Repeat Dose Toxicity</i>	Yes	OECD 422
<i>Developmental Toxicity</i>	Yes	OECD 422
<i>Reproductive Toxicity</i>	Yes	OECD 422
<b>Genetic Toxicity</b>		
<i>Gene Mutation</i>	No	-
<i>Chromosomal Aberration</i>	Yes	OECD 473

## **4.0 PHYSICAL CHEMICAL PROPERTIES**

Physicochemical data (i.e., boiling point, vapor pressure, and log  $K_{ow}$ ) for 2-thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide were determined experimentally.

### **4.1 Boiling Point**

The calculated boiling point for 2-thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide is 362.1°C (Table 1). Experimental measurement is proposed using OECD Guideline 103.

### **4.2 Vapor Pressure**

Modeling data indicate that the vapor pressure of 2-thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide is approximately an 8e-006 mmHg @ 25 °C (Table 1). Experimental measurements are proposed using OECD Guideline 104.

### **4.3 Water Solubility**

The water solubility of thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide determined according to EEC Commission Directive 92/69/EEC Method A6 is 54 mg/L at 20°C. Thus, the calculated and measured values are in close agreement.

### **4.4 Octanol-Water Partition Coefficient**

The log octanol-water partition coefficient (log  $K_{ow}$ ) value of 2-thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide is calculated to be 3.6 (Table 1). Experimental measurements are proposed using OECD Guidelines 117.

## **5.0 ENVIRONMENTAL FATE DATA**

### **5.1 Biodegradability**

The Modified Strum Test (OECD Guideline 301B) was used to evaluate the biodegradability of thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide. After the 28-day test, the extent of biodegradation was 9.6% based on total carbon dioxide production. The available data are adequate and reliable. Additional biodegradation testing will not be conducted.

### **5.2 Hydrolysis**

No published or unpublished hydrolysis studies on thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide were located. The potential for thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide to hydrolyze will be characterized in a technical discussion.

### **5.3 Photodegradation**

No published or unpublished photodegradation studies of thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide were located. The Atmospheric Oxidation Potential (AOP) of this substance will be characterized using the modeling program AOPWIN.

### **5.4 Fugacity Modeling**

No published or unpublished fugacity-based multimedia fate modeling data for thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide was located. The relative distribution among environmental compartments will be evaluated using Level I Fugacity modeling.

## **6.0 ECOTOXICOLOGY DATA**

### **6.1 Aquatic Toxicity**

The 96 hour  $EL_{50}$  of thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide determined in algae is 3.5 mg/L WAF. The NOEL is 0.313 mg/L WAF. The available aquatic toxicity data in algae are adequate and reliable. Additional aquatic toxicity testing in invertebrates and fish is proposed according to OECD Test Guidelines 202 and 203.

## **7.0 MAMMALIAN TOXICOLOGY DATA**

### **7.1 Acute Mammalian Toxicity of Thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide**

Acute oral and dermal toxicity studies are available for thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide. The  $LD_{50}$  in rats (oral) and rabbits (dermal) are >10 g/kg and between 4 and 8 g/kg, respectively. These studies were reviewed and considered reliable. Additional acute mammalian toxicity testing is not proposed.

### **7.2 Mutagenicity of Thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide**

An adequate and reliable bacterial reverse mutation study was performed for thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide. Additional mutagenicity testing for chromosome aberrations will be performed according to OECD Test Guideline 473.

### **7.3 Repeated-dose, Reproductive and Developmental Toxicity of Thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide**

No published or unpublished repeat dose, reproductive or developmental toxicity tests for thiophene, 3-(decyloxy)tetrahydro-, 1,1-dioxide were located. Testing is proposed in the form of OECD Test Guideline 422: A Combined Repeated Dose Toxicity Study with a Reproduction/Developmental Toxicity Screening Test.